AN X-RAY INVESTIGATION ON TETRAPHENYLETHYLENE CRYSTAL*

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ABSTRACT A systematic study of X-ray reflections from a large number of planes, indicates that the space group of this crystal is P_2/m. The estimated intensities of these planes show that the molecule does not lie in any simple crystallographic plane.

In the previous communication (Datta, 1953), we have seen that the crystal of tetraphenylethylene belongs to monoclinic holo-axial system. Morphological study and three rotation photographs about the three crystallographic axes using Ni-radiation gave the following values for the axial lengths and angles

$$a = 11.30 \text{ Å}.$$
$$b = 9.37 \text{ Å}.$$
$$c = 10.10 \text{ Å}.$$
$$\beta = 72^\circ$$

b-axis is the axis of symmetry and β is the angle between a and c axes. The density of the crystal (by floatation method) was found to be 1.057. On substitution of these values in the formula

$$N = \frac{\rho V}{A M_H}$$

where N = No. of molecule per unit cell, ρ = density, V = volume, A = at weight. M_H = mass of hydrozen atom, the number of molecules per unit cell was found to be one. Hence the crystal has neither glide plane nor screw axis.

This is further confirmed by identifying a large number of reflecting planes on oscillation photographs. The b-axis of the crystal was made vertical. Oscillation photographs were taken over 10° oscillation. 18 photographs were taken from 0° to 180°. The spots were identified (usual method, Banerjee and Singh, 1937) on reciprocal lattice network of a^* and c^*. The relative intensities as determined by eye-estimation, were noted down against all the spots.

From the Table (Astbury and Yardley) it is shown that

all (hol) planes are present

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so that *b*-axis is the axis of symmetry, and (*a*, *c*) plane is the plane of symmetry. There are a few absent spectra which are due to symmetrical arrangement of phenyl groups themselves. The space group of the this crystal will be, therefore, $P2/m$.

In the previous communication (Datta, 1953), we have seen that the crystal is bi-axial and optically negative with

$$\alpha = 1.690,$$
$$\beta = 1.757,$$
$$\gamma = 1.762.$$

The lowest refractive index being normal to the plane of molecule (Datta, 1947), since the above values are nearly equal, the molecule does not lie in any simple crystallographic plane. Our estimated intensities also support this view. Therefore, the complicated molecule as it is will not be planar.

TABLE I

The following planes have been identified.

Planes	Intensity	Planes	Intensity
002	S	313	V.S.
003	V.S.	314	W
004	S	315	W
005	W	400	S
010	S	401	W
012	V S.	402	S
013	V S.	403	S
014	S	404	W
020	V S.	500	V.S.
022	V.S.	501	V.W
023	S	502	S
024	S	303	W
025	S	504	W
030	V.S.	505	V.W.
032	S	600	W
033	W	601	W
033	W	603	S
100	S	604	S
101	S	606	S
102	S	701	W
103	W	702	W
104	V V W	703	W
105	S	704	W
200	V.S	803	V W.
201	S	805	W
202	S	807	W
203	S	903	V W.
204	W	905	V.V.W
205	S	10 02	S
301	V.S.	110	V.W.
302	W	111	V.S.
303	W	112	V.S.
304	S	115	S
311	W	113	W
312	W	114	V.W.

TABLE I (contd.)

Planes	Intensity	Planes	Intensity
121	S	515	
122	V S	610	V.W.
123	S	611	W
124	V S	613	W
125	W	614	V.V W.
130	V.S	711	W
131	S	712	W
132	W	713	S
133	S	714	W
134	V S	815	W
211	S	915	S
212	S	420	S
213	S	421	W
214	V S	422	W
213	W	423	V.W.
220	S	424	W
221	S	520	S
222	V S.	521	S
223	S	522	S
224	S	523	S
225	S	524	W
231	S	525	V.W.
232	S	620	W
233	S	621	S
234	S	623	W
235	W	624	W
321	W	724	W
322	S	821	W
320	S	825	W
323	S	430	S
324	W	431	V.W.
531	S	432	S
332	W	433	V.W.
333	S	434	S
410	S	530	V.W.
411	S	531	S
412	V.S	532	S
413	W	533	W
414	W	534	W
510	S	630	W
511	S	633	W
512	S	634	W
513	W	734	W
514	W	835	W

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